BERKELEY LAB
Bringing Science Solutions to the World

U.S. DEPARTMENT OF ENERGY

Recommendations for Data Management

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2019 AmeriFlux Data-Tech Workshop

October 29-30, Berkeley, CA

AMERIFLUX
MANAGEMENT PROJECT

Outline

- **Checklists:** *no one is too cool for school*
- **Data Lifecycle:** before that one file disappears…
- **Data Management Best Practices:** pick yours now!
  - AmeriFlux resources
- **What's on your checklist?**

Surgery staff

Aircraft pilots

Surgery sta

rcraft pilots

Both were initially resistant/skeptical towards adopting checklists into work routines

Surgery sta

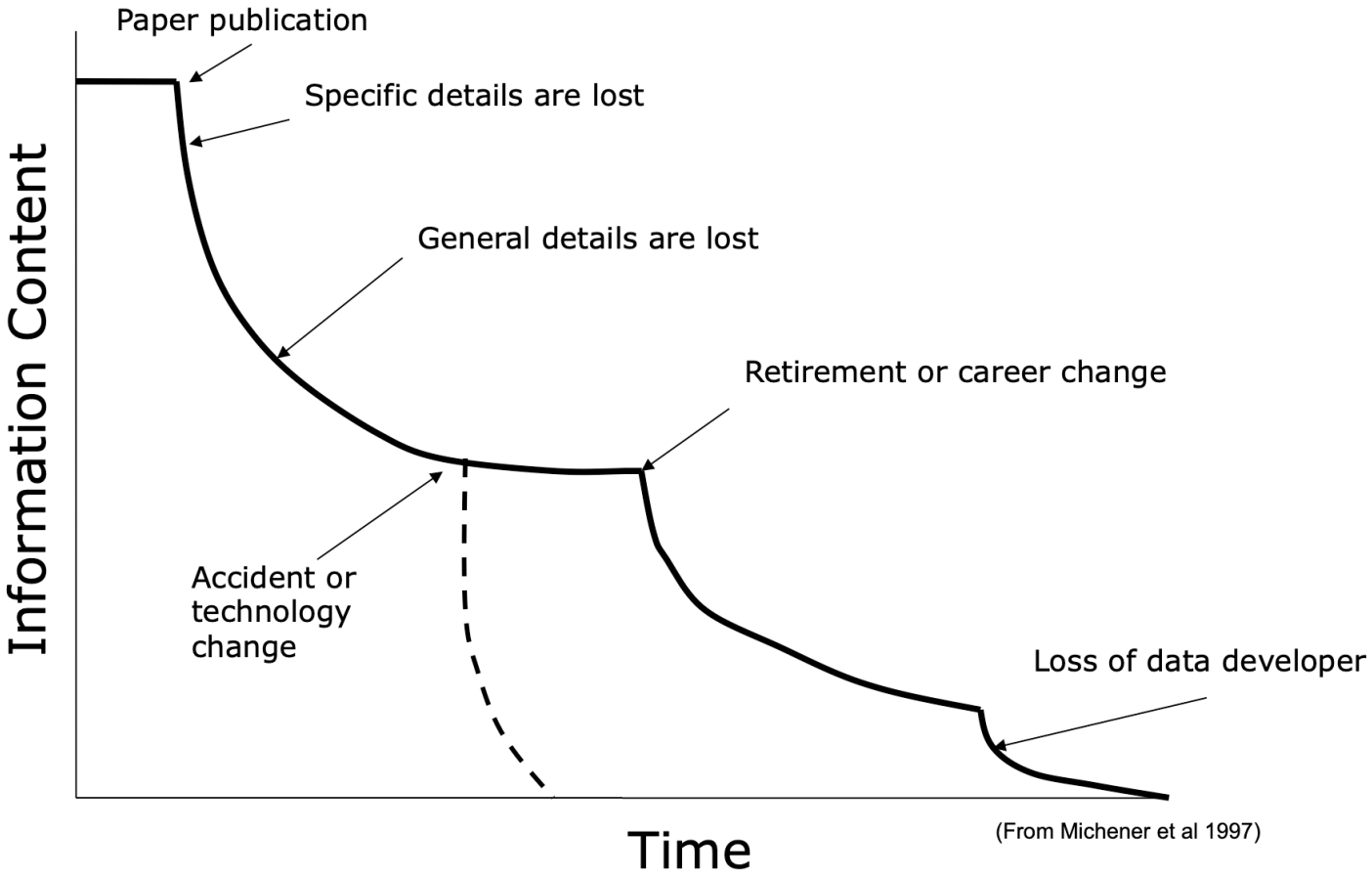
rcraft pilots

Both were initially resistant/skeptical towards adopting checklists into work routines

*Recommendation: **Hidden Brain** episode on checklists (NPR podcast, hosted by Shankar Vedantam)*
https://www.npr.org/2017/10/30/559996276/the-trick-to-surviving-a-high-stakes-high-pressure-job-try-a-checklist

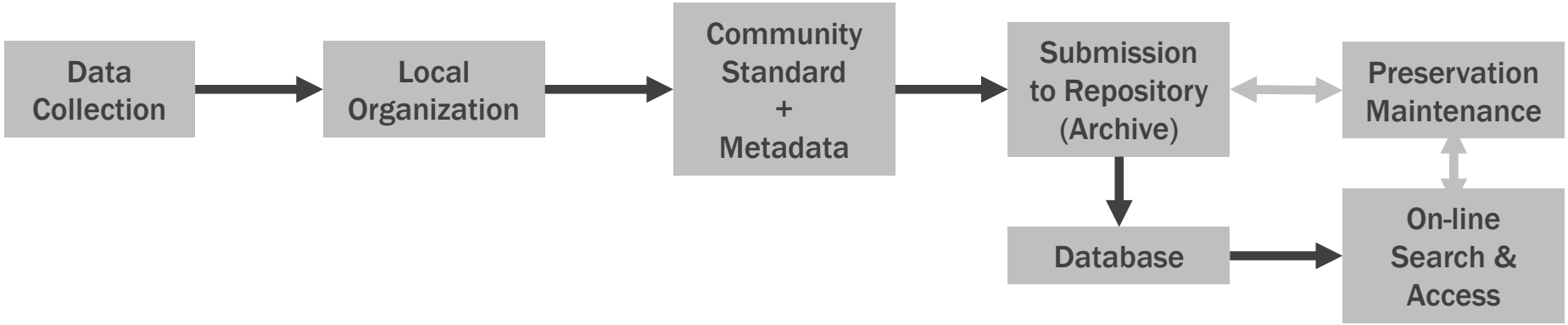
Why Think About Data Lifecycle

Information Entropy



(From Michener et al 1997)

Good data management involves entire Data Lifecycle



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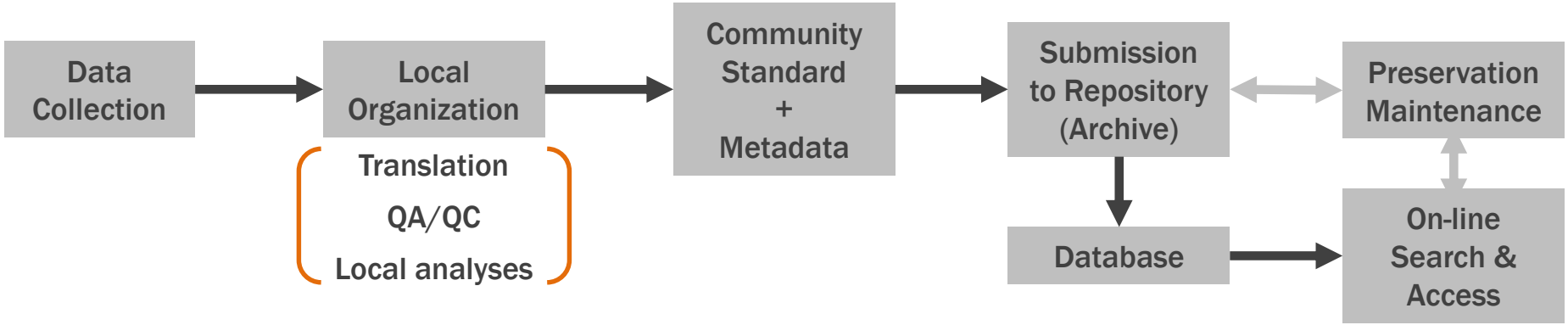

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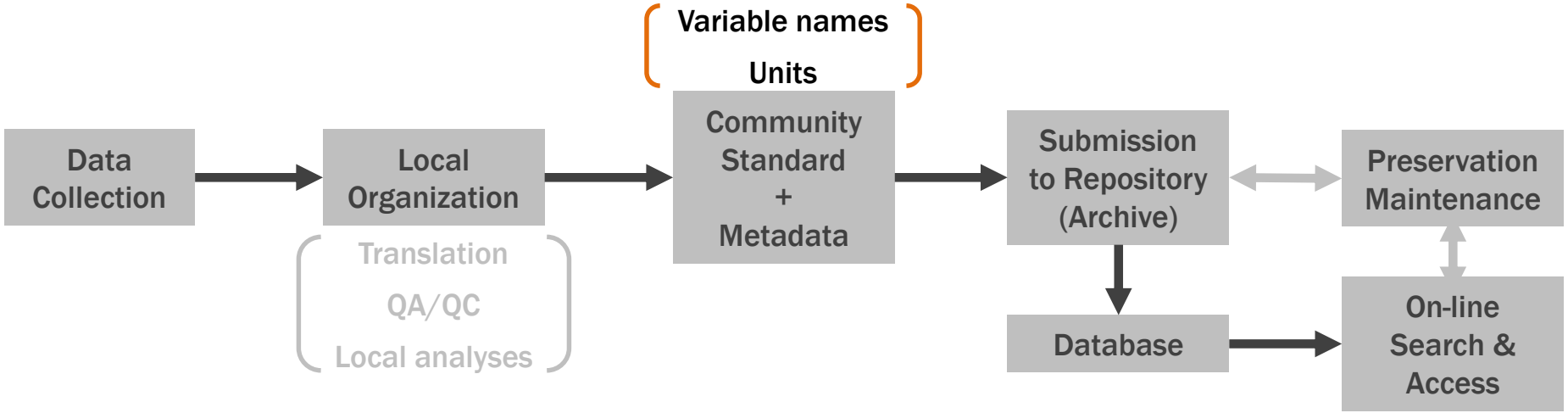

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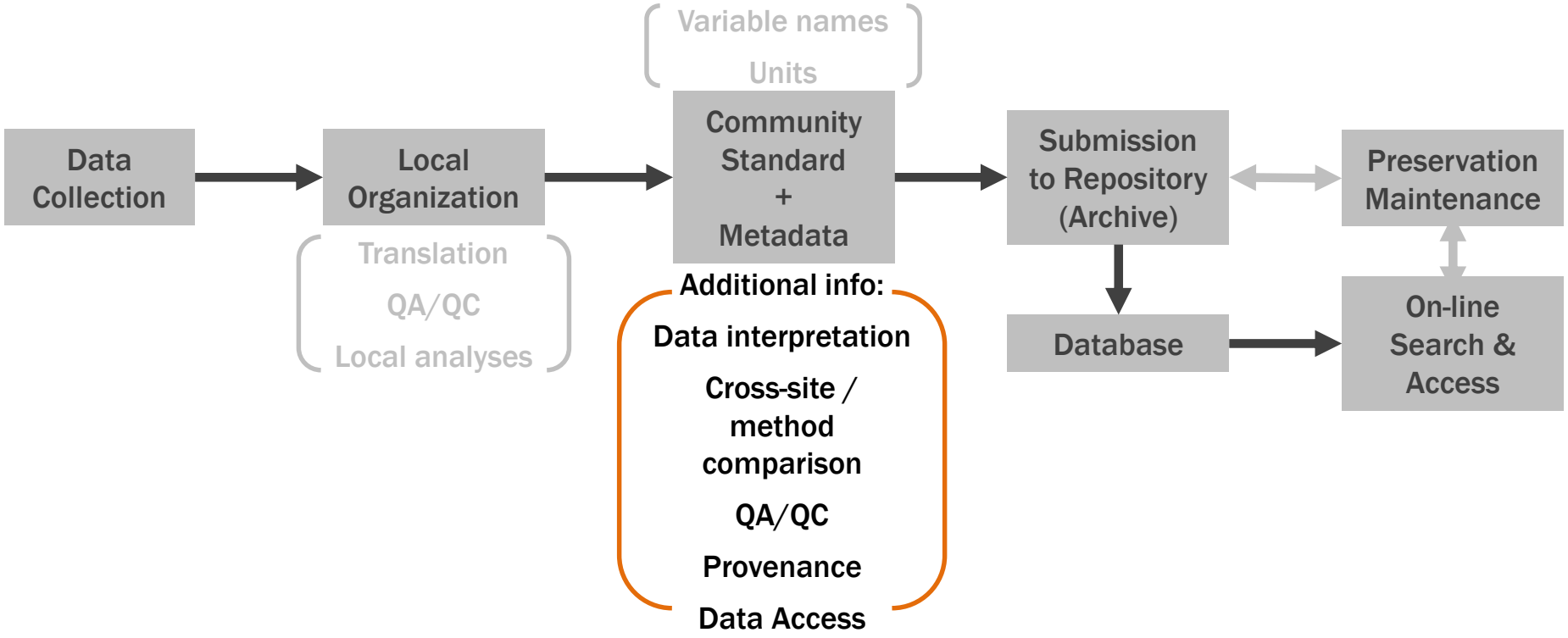

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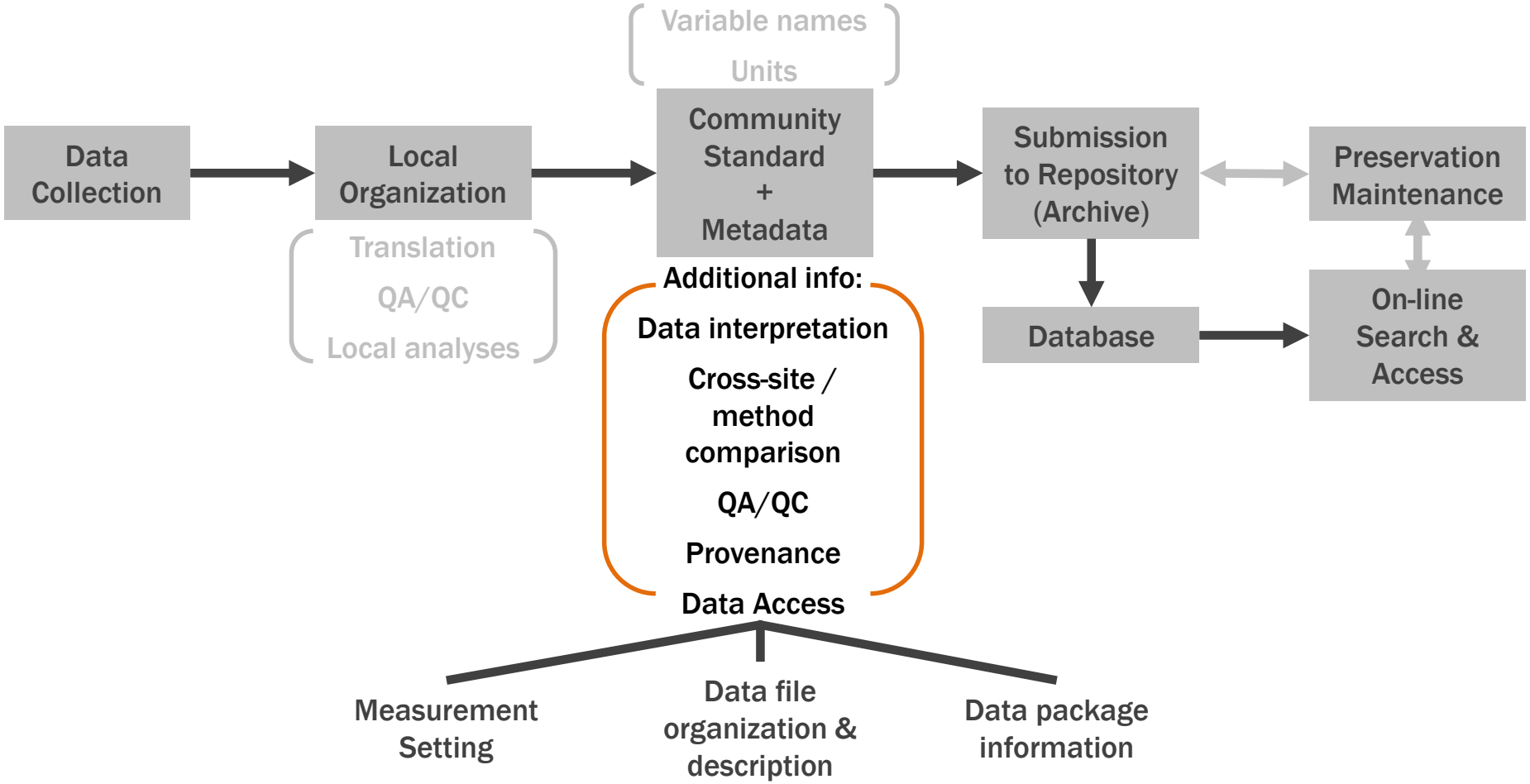

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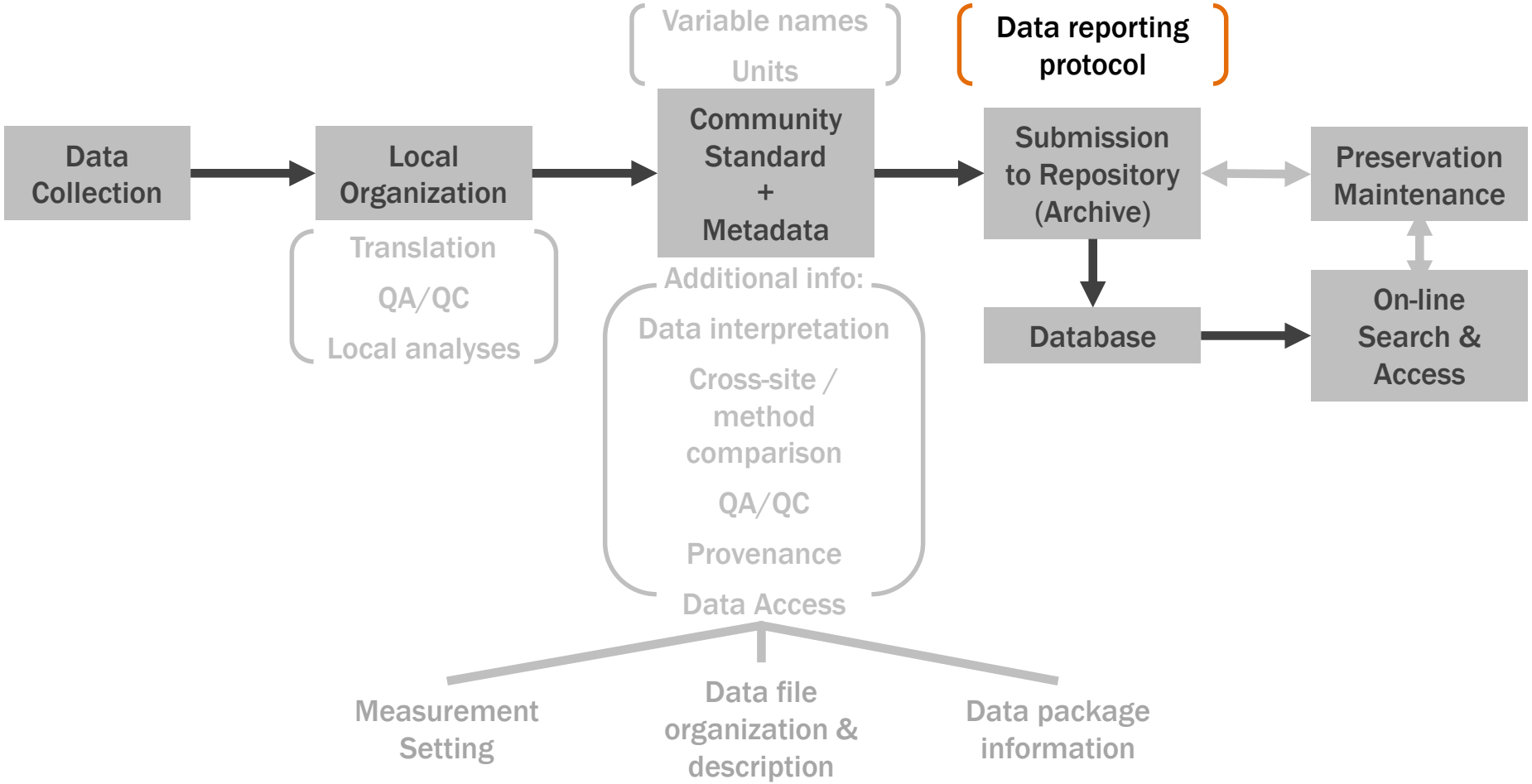

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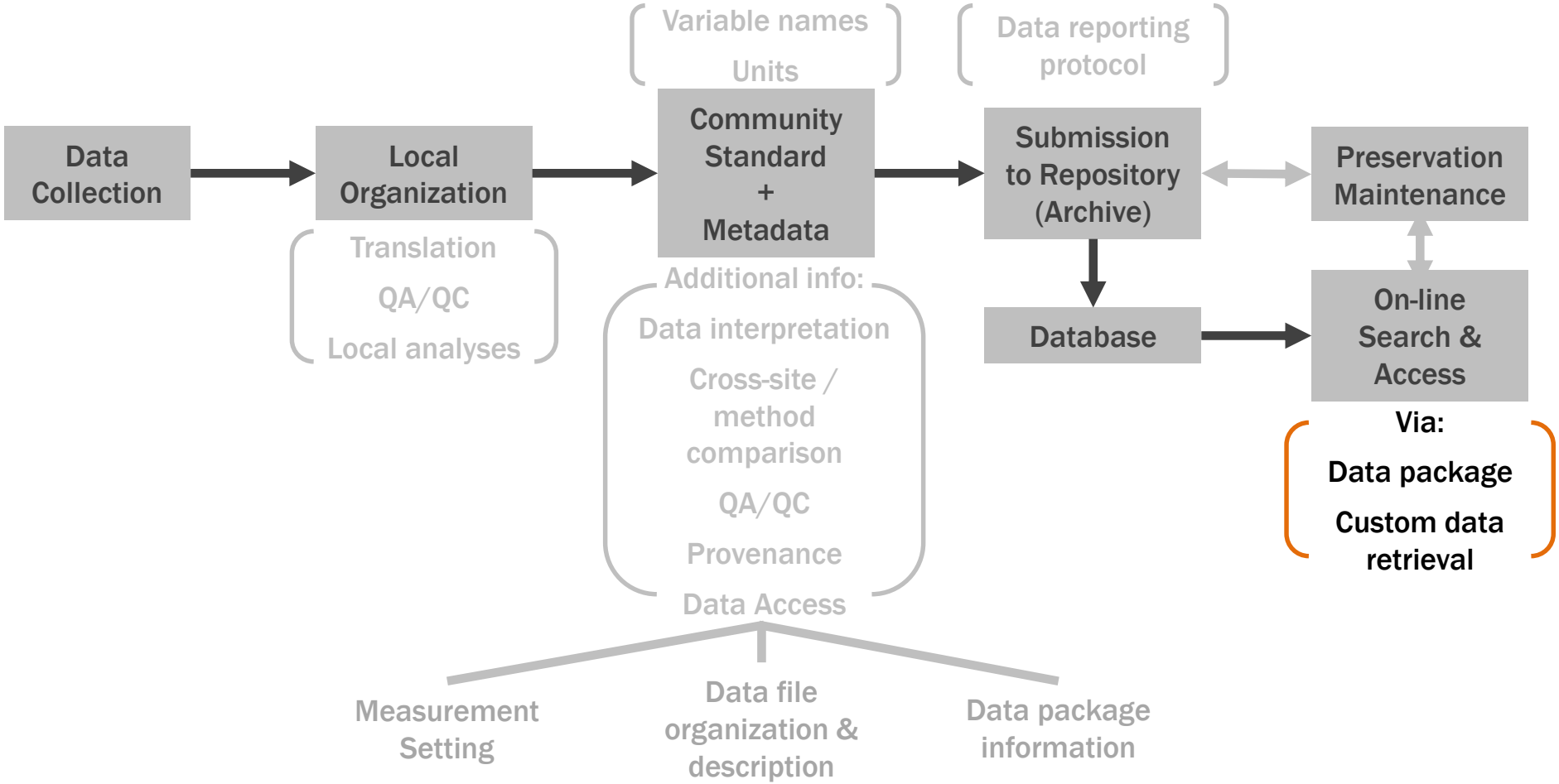

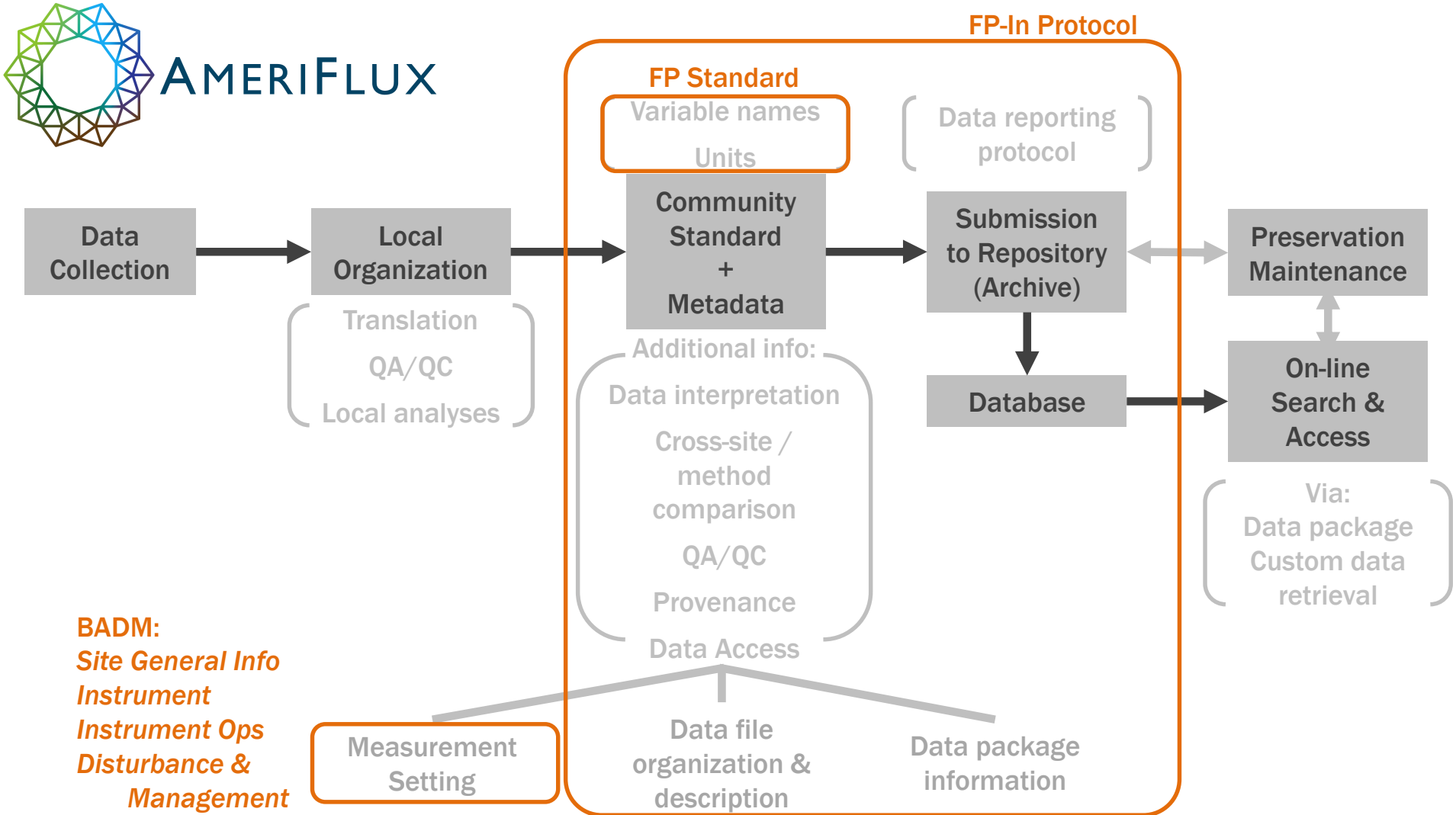
AMERIFLUX
FP-In Protocol
FP Standard
Variable names
Units
Data reporting protocol
Data Collection
Local Organization
Community Standard + Metadata
Submission to Repository (Archive)
Preservation Maintenance
Translation
QA/QC
Local analyses
Additional info:
Data interpretation
Cross-site / method comparison
QA/QC
Provenance
Data Access
Database
On-line Search & Access
Via:
Data package
Custom data retrieval
BADM:
Site General Info
Instrument
Instrument Ops
Disturbance & Management
Measurement Setting
Data file organization & description
Data package information

AMERIFLUX

https://ameriflux.lbl.gov/data/aboutdata/data-variables/

2. Data Variable: Base names

Base names indicate fundamental quantities that are either measured or calculated / derived. They can also indicate quantified quality information.

Table 1. Base names for data variable labels

Name	Description	Units
TIMEKEEPING		
TIMESTAMP_END	ISO timestamp end of averaging period (up to a 12-digit integer as specified by the data's temporal resolution)	YYYYMMDDHHMM
TIMESTAMP_START	ISO timestamp start of averaging period (up to a 12-digit integer as specified by the data's temporal resolution)	YYYYMMDDHHMM
GASES		
CO2	Carbon Dioxide (CO2) mole fraction	µmolCO2 mol-1
H2O	Water (H2O) vapor mole fraction	mmolH2O mol-1
CH4	Methane (CH4) mole fraction	nmolCH4 mol-1
NO	Nitric oxide (NO) mole fraction	nmolNO mol-1
NO2	Nitrogen dioxide (NO2) mole fraction	nmolNO2 mol-1
N2O	Nitrous Oxide (N2O) mole fraction	nmolN2O mol-1
O3	Ozone (O3) mole fraction	nmolO3 mol-1
FC	Carbon Dioxide (CO2) turbulent flux (no storage correction)	µmolCO2 m-2 s-1
FCH4	Methane (CH4) turbulent flux (no storage correction)	nmolCH4 m-2 s-1

AMERIFLUX

https://ameriflux.lbl.gov/sites/siteinfo/CC-SSS

BADM Editor: Site General Info

US-Ton: Tonzi Ranch

* *indicates required field*

get more information

GRP_TEAM_MEMBER

Add New Entry

TEAM_MEMBER_NAME
Dennis Baldocchi

TEAM_MEMBER_ROLE
PI

TEAM_MEMBER_EMAIL
Baldocchi@berkeley.edu

TEAM_MEMBER_INSTITUTION
University of California, Berkeley

TEAM_MEMBER_ADDRESS
Department of Environmental Science, Policy and Management, 137 Mulford Hall, 345 Hilgard Hall,Berkeley, CA USA 94720-3110

TEAM_MEMBER_NAME
Siyan Ma

TEAM_MEMBER_ROLE
FluxContact

TEAM_MEMBER_EMAIL
syma@berkeley.edu

TEAM_MEMBER_INSTITUTION
University of California, Berkeley

TEAM_MEMBER_ADDRESS

TEAM_MEMBER_NAME
Joe Verfaillie

TEAM_MEMBER_ROLE
Technician

TEAM_MEMBER_EMAIL
jverfail@berkeley.edu

TEAM_MEMBER_INSTITUTION
University of California, Berkeley

TEAM_MEMBER_ADDRESS

GRP_SHIPPING_ADDRESS

AMERIFLUX

https://ameriflux.lbl.gov/data/badm-data-templates/

Variable	Description	Units
SITE_ID	Six character site identifier. MANDATORY if site is already registered	CC-Xxx
SITE_NAME	Site name	free text
SUBMISSION_CONTACT_NAME	Name of person who submitted this template	free text
SUBMISSION_CONTACT_EMAIL	E-mail address of the person who submitted this template	free text
SUBMISSION_DATE	Date this submission was last edited/modified.	YYYYMMDD
INST_MODEL	Manufacturer and model	LIST(INST_MODEL)
INST_SN	Serial number or other unique text string used to identify this instrument	free text
INST_DESC	Instrument description, include model if INST_MODEL is "other"	free text
INST_INSTALL_TYPE	Instrument installation type : new deployment, redeployment at different location, temporary loaner	LIST(INST
INST_INSTALL_DATE	Instrument installation date	YYYYMMI
INST_FIRMWARE	Instrument firmware version at installation	free text
INST_HEIGHT	Meters above/below groundfrom site reference point at ground level (negative values: below ground)	m
INST_EASTWARD	Distance E-W from the site reference point. Negative values are West from tower reference point.	m
INST_NORTHWARD	Distance N-S from the site reference point. Negative values are South from tower reference point.	m
INST_SAMPLING_INT	Sampling interval at datalogger	seconds
INST_AVERAGING_INT	Averaging interval for data from data logger if different from sampling interval	seconds
INST_HEAT	Instrument heating	LIST(INST
INST_SHIELDING	Instrument shielding such as radiation or rain; use "none" if not shielded.	LIST(INST
INST_ASPIRATION	Instrument aspiration such as natural or mechanical; use "none" if not aspirated.	LIST(INST
INST_ANEM_OFFSET_NORTH	Orientation of the instrument from magnetic north. Only positive values 0-359 degrees.	degrees (
INST_ANEM_WIND_FORMAT	Format for wind components are reported	LIST(ANE
INST_ANEM_GILL_ALIGN	North aligment for Gill brand anemometers	LIST(ANE
INST_REF_ANEM_MODEL	The reference anemometer model	LIST(INST

vocabulary	shortname	description
ANEM_ALIGN_NORTH	Spar	Spar is oriented North
ANEM_ALIGN_NORTH	Axis	Axis is oriented North
ANEM_ALIGN_NORTH	NA	Not Applicable
ANEM_WIND_FORMAT	U, V, W	2D horizontal, 1D vertical
ANEM_WIND_FORMAT	Polar and W	Horizontal angle and vertical
ANEM_WIND_FORMAT	Axis	Axis velocities
GA_CP_MATERIAL	Teflon	Teflon tube
GA_CP_MATERIAL	Iron	Iron tube
GA_CP_MATERIAL	Glass	Glass tube
GA_CP_MATERIAL	Other	Other type of tube
GA_CP_THERMAL	Insulated	Insulation only
GA_CP_THERMAL	Heated	Heating installed
GA_CP_THERMAL	None	No thermal treatment
INST_ASPIRATION	Ventilation	
INST_ASPIRATION	Mechanical	
INST_ASPIRATION	None	
INST_HEAT	Unheated	
INST_HEAT	Heated	
INST_INSTALL	new installation	First intallation of an instrument at the site
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INST_MODEL	SA-ATI SATI A Style	Sonic Anemometer - ATI SATI A Style
INST_MODEL	SA-ATI SATI K Style	Sonic Anemometer - ATI SATI K Style
INST_MODEL	SA-ATI Sx Style	Sonic Anemometer - ATI Sx Style

AMERIFLUX

https://ameriflux.lbl.gov/data/upload-data/

Upload Data: Half Hourly

< Back

To submit Ameriflux data file(s), please:

- Make sure that your data is in standard Ameriflux format
- Select options below and upload the file(s)

Select Site *

Selected Site: **None** | Type Site ID or name...

BR-Ma2: Manaus - ZF2 K34

BR-Sa1: Santarem-Km67-Primary Forest

BR-Sa3: Santarem-Km83-Logged Forest

CA-Ca1: British Columbia - 1949 Douglas-fir stand

I do not have a Site ID

Gap Filling *

No gaps are filled

Some or all gaps are filled

Data File(s) to Upload *(200 MB size limit per file)

Add File(s)

Description *

Notes about this data upload. These notes help us process the data correctly.

File Containing Description of this Upload

Add File

By clicking Upload, I acknowledge that I have read and agreed to the Ameriflux Data Policy.

Upload | Clear All Files

If you have questions, please contact us at ameriflux-support@lbl.gov. For more information see About Data and How to Upload/Download Data.

Recommendations for Data Management

- A checklist
  (not the checklist…)

1. Value

- Data as an actual product of research, not only as a means to publish papers
- A data set has value by itself and as a future “commodity” for other studies
- Interest in a data set by itself and combined with others

2. Metadata

- Metadata before even starting *(mostly applicable to data collection efforts)*
- Machine-readable
  - format
  - structure
  - value ranges
  - standards
- Human-understandable
  - describe fields (dictionary of fields)
  - describe potential meaning of missing values
- From an automation perspective:
  - Structured (search, filter, browse, etc)
  - Free text (search only)
- Standards
  - Ecological Metadata Language (EML)
  - Geography Markup Language (GML)
  - **BADM**

2. Metadata

Variable	Description	Units
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INST_MODEL	SA-ATI V Style	Sonic Anemometer - ATI V Style
INST_MODEL	SA-ATI Vx Style	Sonic Anemometer - ATI Vx Style
INST_MODEL	SA-ATI CATI/2	Sonic Anemometer - ATI CATI/2
INST_MODEL	SA-ATI SPAS	Sonic Anemometer - ATI SPAS
INST_MODEL	SA-ATI	Sonic Anemometer - ATI
INST_MODEL	SA-Campbell CSAT-3	Sonic Anemometer - Campbell CSAT-3
INST_MODEL	SA-Gill HS-50	Sonic Anemometer - Gill HS-50
INST_MODEL	SA-Gill HS-100	Sonic Anemometer - Gill HS-100

3. Organization

- File system
  - folder structure
  - metadata location and granularity
- Database
  - schema definition
  - accommodation of changes
- Changes to organization
  - reformat everything
  - document differences in organization and attach description to both previous and new organizations

4. File Formats

- Text (CSV): easy to use; requires care for machine readability
- Binary: open, royalty-free, well documented
- Hardware format concerns:
  - Longevity of format (floppy disk, optical disk, spinning disk, flash memory, magnetic tape, etc.)
  - Readability of format
  - Cloud storage
  - “Keep alive” approach usually best

5. Rows vs Columns

- For manual editing column-long formats can be easier
  - avoid changing column orders

date	var1	var2	var3	var4
20190607	10	20	30	40
20190608	11	21	31	41

date	variable	value
20190607	var1	10
20190607	var2	20
20190607	var3	30
20190607	var4	40
20190608	var1	11

- For automated use (databases, software), row-long format can be more flexible (simplify queries, more flexible to changes)

6. Data Types

- File headers: non-numerical types
- Data cells: numerical-only, text, date/time
- Complex / simple types:
  - Readability
  - Compactness

7. Date / Time

- Consistent formats
- Standard formats
  - ISO 8601
    - YYYYMMDDhhmmss
    - YYYY-MM-DDThh:mm:ss

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- Consistent formats
- Standard formats
  - ISO 8601
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AMERIFLUX

8. Responsibilities

- Role to be filled for data management: clear identification of responsibilities
- Helps answer data related issues and can enforce compliance
- Shared responsibility still requires clear identification of tasks/data

9. Budgets

- Financial budget for data management
  - equipment
  - media
  - work hours
- Time budget for data management
  - allocated time for periodic housekeeping
  - allocated time for milestone handling

10. Backup

- Raw data goes first
- Keep key versions and use clear labels
- Periodicity
  - full, differential, incremental
  - unchangeable copies (raw, milestones)
  - “Work on” copies
  - multiple versions
- Physical location of copies
- Size limitations (use documentation to compensate)
- TEST YOUR BACKUP!

10. Backup
AmeriFlux backup service

- All site relevant data
  - **High-frequency data** (IRGAs and Sonics)
  - Micrometeorological data (any/original frequency)
  - Processed data
  - Field notebooks
  - Pictures
- Backup only, data not made available to anyone besides site team

https://ameriflux.lbl.gov/data/how-to-uploaddownload-data/uploading-high-frequency-data/

10. Backup
AmeriFlux backup service

- High Frequency Data
  - Format
    - Currently no formal specifications (experiments and feedback will guide)
    - Experience from site teams, AMP Tech Team, and ICOS protocols
  - What to send:
    - Closest as possible to output from data acquisition system (no/little processing) – site owned reproducibility
    - QA/QC'd version also encouraged

10. Backup
AmeriFlux backup service

- Uploading data Data
  - Secure Copy / Secure FTP data transfer protocol
  - Steps:
    1. Generate SSH key pair (public/private)
    2. Send us public SSH key
    3. Start uploading data

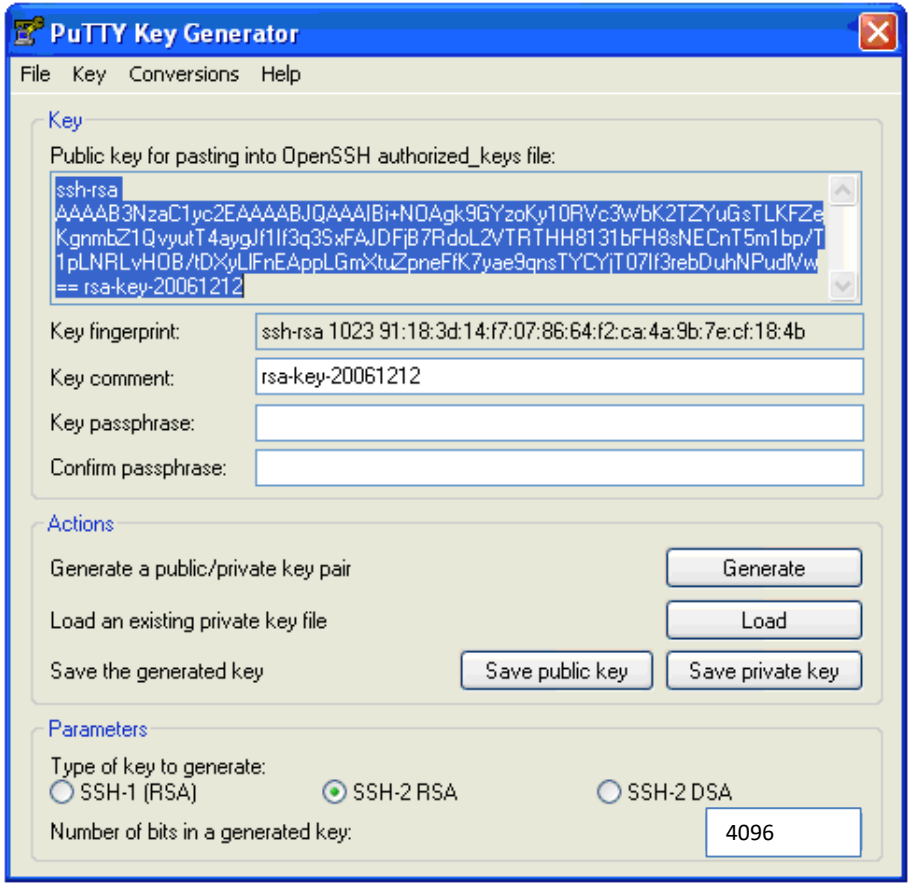
Generate SSH Key (Linux/Mac)

$ ssh-keygen -t rsa -b 4096 -f /PATH/TO/KEYS/KEY

```
Last login: Tue Sep 20 09:09:53 on ttys004
gilberto@rl1gw2-197-209-dhcp.int.colorado.edu:~$ ssh-keygen -t rsa -b 4096 -f /tmp/testkey
Generating public/private rsa key pair.
Enter passphrase (empty for no passphrase):
Enter same passphrase again:
Your identification has been saved in /tmp/testkey.
Your public key has been saved in /tmp/testkey.pub.
The key fingerprint is:
07:e8:d1:b7:14:a0:73:e8:c6:76:89:24:1c:61:ef:d3 gilberto@rl1gw2-197-209-dhcp.int.colorado.edu
The key's randomart image is:
+--[ RSA 4096]----+
|    +.  ...       |
|   o o =   .      |
|    o O + o       |
|     B * = .      |
|      X E o       |
|     o o .        |
|                  |
|                  |
|                  |
+-----------------+
gilberto@rl1gw2-197-209-dhcp.int.colorado.edu:~$
```

Generate SSH Key (Windows)

PuTTY Key Generator: puttygen.exe



Send us the **Public** SSH Key

Public Key (send us):


```
---- BEGIN SSH2 PUBLIC KEY ----
Comment: "Ameriflux SITE [2048-bit rsa, useremail@email.com, Wed Mar 18 2015 07:31:32]"
AAAAB3NzaC1yc2EAAAADAQABAAABAQCgQBYh8pzsBzhqgmfiOG0X4qsu49obwERr
X9LtcI2KZDQbYz4U/mlq5OoUWUIkXRsXT5GawCyzxp7wZvu5LeC3PSoLyY3FRKcM
rvdxRUjdVTTSnGftfO6rLDGFJGL5DNB/Xdsg/d9Z6bIsT8Cit1Hb+ZsvEMYbhVE8
X9LtcI2KZDQbYz4U/mlq5OoUWUIkXRsXT5GawCyzxp7wZvu5LeC3PSoLyY3FRKcM
tzUcaQEcVSuDtNI4hS1DcElCHTTxSWgszrCqczp9FLTRL+qBNU/6JsNgJ0L5YCJS
EAAAADAQABAAABAQCgQBYh8pzsBzhqgmfinjuXg5bm9p8zDYta+L1
---- END SSH2 PUBLIC KEY ----
```


Private Key (keep it safe):


```
-----BEGIN RSA PRIVATE KEY-----
Proc-Type: 4,ENCRYPTED
DEK-Info: AES-128-CBC,7EA12B1B2794E57704BB622E4D3E11DD

yo5lxQ6QDVn9HRTXSTQhPANkZiSjBanL0pMkgV9aA3HvgRshQG535T
TUSegJq/WOfinLr7jWV4NYj8tL8M4Xi0X0oEG3XRYChFnVn7KJM6t6
LKq2SKrYQLbjADVY27FJakwOiOTL1UC46vRXRZkHUG0XgGYWrCnc2U
. . .
CF+SPqAy3MH8J9h10oqPcYHuvvQNvBZE5ACjdpomfzm7X4efAOPAMO
RIMjRnaKkyEZpAOs0k57Nz8AyMSnwrkEdvIcRB/dQhox6WgTyS6lcM
g6+xLYL9ijM12sPvJzR8H1MvzGAsPNNnhkVMUrUXvCEBDAhOyg0HC1
-----END RSA PRIVATE KEY-----
```


One SSH Key (pair) per site

Send us the **Public** SSH Key

- Public Key file: my-key-filename**.pub**

- Upload:

http://ameriflux.lbl.gov/data/upload-data/

- Email:

ameriflux-support@lbl.gov

Upload data

- Windows:

```
C:\> c:\PATH\TO\PSCP\pscp.exe
    -i c:\PATH\TO\KEYS\KEY.ppk
    -scp c:\PATH\TO\DATA\DATAFILE.DAT
    fluxnet@dtn01.nersc.gov:
```

Upload data

- Windows:

```
C:\> c:\PATH\TO\PSCP\pscp.exe
    -i c:\PATH\TO\KEYS\KEY.ppk
    -scp c:\PATH\TO\DATA\*
    fluxnet@dtn01.nersc.gov:
```

Upload data

- Linux/Mac:

```
$ scp
  -i /PATH/TO/KEYS/KEY
  /PATH/TO/DATA/*
  fluxnet@dtn01.nersc.gov:
```

Download Data Backups

- Contact us to restore a backup
- More flexible mechanisms planned

11. Software

- Documentation
  - In code comments
  - Clear references to papers and methods
  - Short descriptions at all levels (package, module, function, complex lines)
- Modules
  - Division into logical blocks of: files, functions, etc.
- Versions
  - Version control

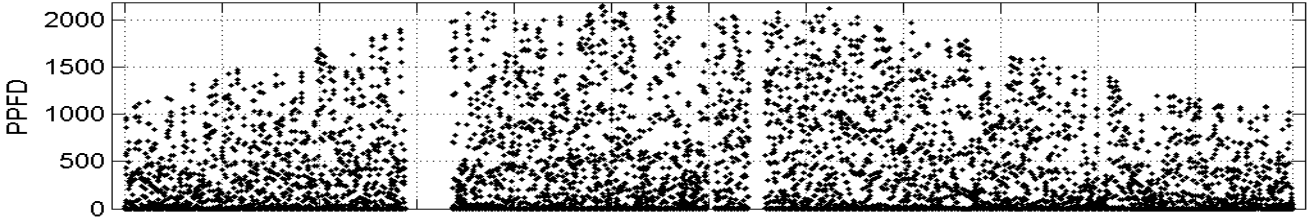
12. Look at the data

- Time series data, time series plot:
  - **Full time series**, year, month, days

- Distribution plots
  - Trends with hidden periodicity
  - “Common” distribution for a site / season

12. Look at the data

Example: Time Scales



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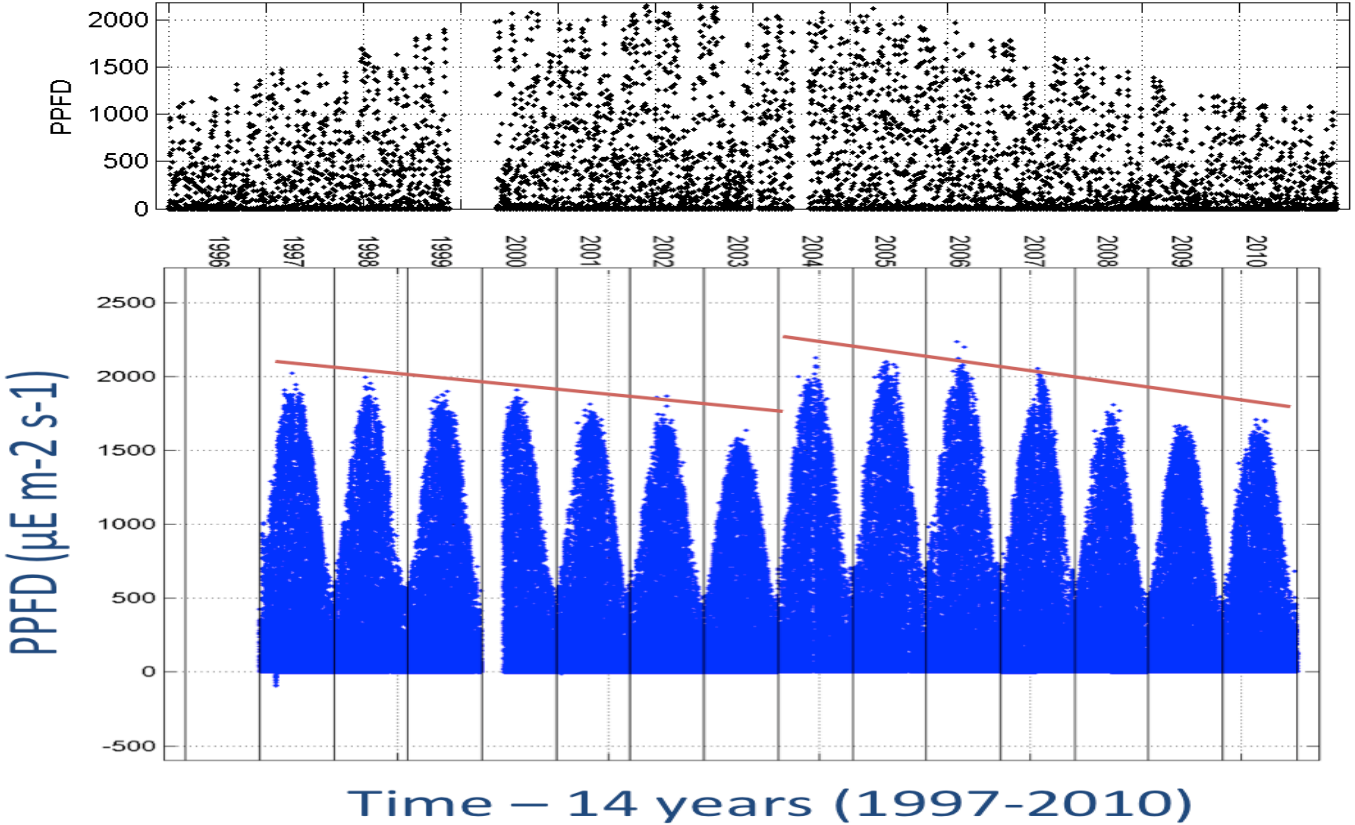

13. Sharing

- Terms of Sharing, Use, Licenses
- Archival
- Publication (of data and “data paper”)
  - Time spent working on data
  - Research results and artifacts

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14. 10-year Documentation

- When going through all previous practices, consider a 10 years scenario:
  Suppose you try to use your own data again 10 years after it was used last. Will you be able to do it with your choices in practices?

- Have a 10 year-resistant mind set for data documentation

Checklists **must have** a **TL;DR** version

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- ❑ 1. Recognizing data value
- ❑ 2. Creating/maintaining metadata
- ❑ 3. Using consistent and sane data organization
- ❑ 4. Selecting appropriate file formats
- ❑ 5. Taking advantage of Rows vs Columns representations
- ❑ 6. Being aware of and using good data types (“no type” can be an option)
- ❑ 7. Using conventions for timestamps
- ❑ 8. Dividing and following-up on data responsibilities
- ❑ 9. Including data management in project budgets
- ❑ 10. Having and testing a backup plan
- ❑ 11. Following Software Development best practices
- ❑ 12. Looking at the data at all steps of the pipeline
- ❑ 13. Making data sharing an integral part of the data activity
- ❑ 14. Creating a 10-year resistant data plan

BONUS: Data Management Plans

- Describes the **types of data**, samples, physical collections, software, data products, and other materials to be produced
- Identifies the **standards to be used for data and metadata** format and content
- Describes the plans for **storing, versioning, and curating data** and making it available for access and sharing
- Defines **policies for access and sharing data** including provisions for appropriate protection of privacy, confidentiality, security, intellectual property, or other rights or requirements inherent in the data
- Identifies **plans for archiving data**, samples, and other research products, and what data will be preserved as well as plans for long-term access to the data
- Defines **who is responsible** for execution of the data management plan

BONUS: Data Management Plans

- Describ
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- Identifi
content
- Describ
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- Defines
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- Identifi
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the data
- Defines

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plan

How is all this reflected on *your checklist* (a.k.a., the **actual** Data Management Plan)

Questions? Comments? Suggestions?

What's on your checklist?

contact: ameriflux-support@lbl.gov

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